

TRANSITION PROBABILITIES FOR SEVERAL INFRARED LINES OF Tl I AND Ar I

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Abstract—Relative transition probabilities for 18 infrared (i.r.) lines arising from excited doublets levels of Tl I and 68 lines belonging to the Ar ($4p-3d$), ($4p-5s$) and ($4s-4p$) transition array, and coming from the upper levels $3d[3/2]_1$, $3d[7/2]_3$, $3d[5/2]_2$, $3d'[3/2]_2$, $3d'[5/2]_2$, $3d'[3/2]_1$, $5s'[1/2]_0$, $5s[3/2]_1$, $5s[3/2]_2$, $4p[1/2]_1$, $4p[5/2]_2$, $4p[3/2]_1$, $4p[3/2]_2$, $4p'[3/2]_1$, $4p'[3/2]_2$ and $4p'[1/2]_1$ (jK notation), have been determined from emission line-intensity measurements of an optically-thin light source. Transition probabilities were placed on an absolute scale by using line-strength sum rules. Our experimental results are compared with experimental and theoretical data, where possible, given by other authors. ¹

INTRODUCTION

Relative transition probabilities for $7s-np$, $6p-ns$ and $6p-nd$ i.r. lines of Tl I have been the subject of numerous theoretical studies using a variety of simple models which have been based on the one-electron central-field approximation, Anderson et al.,¹ Migdalek,² Neuffer and Commins³ and Bardsley and Norcross⁴ among others; for these lines there are no published experimental studies, and this situation has prompted the present measurements. In this study I also give transition probabilities for 68 i.r. lines of Ar I which are the subject of few experimental and theoretical studies.

The method used to determine transition probabilities was similar to that employed in previous studies.⁵⁻⁷ We measured emission intensities of lines arising from the same upper level to determine relative transition probabilities, whose values become independent of the upper level population when working with optically-thin light sources.⁸ Transition probabilities are obtained on an absolute scale by using line-strength sum-rules,⁹ and the Coulomb approximation for i.r. lines of Ar I. The results are compared with the intermediate-coupling calculation of Lilly,¹⁰ who also used the Coulomb approximation, as well as with previously published experimental results of Wiese,^{11,12} Tanarro^{5,6} and Borge.¹³

Tl I transition probabilities also have been obtained on an absolute scale by using line-strength sum-rules and relativistic semiempirical method which included core-polarization effects, both in the model potential and in the transition matrix element. These experimental results are compared with theoretical calculations performed by other authors. To provide level energies of our calculations, the tables of Moore¹⁴ have been used.

EXPERIMENTAL SET-UP AND PROCEDURE

The experimental set-up is similar to that described in a previous publication.^{7,15} The spectral source used was an a.c. Tl arc lamp operating at 0.9 A, and the light path was 1 cm, the gas used to fill the tube was Ar at a pressure of 1 torr. The wavelengths of the measured transition are in a range from 7000 to 15,000 Å; the lines were selected by means of a 1 m Eagle monochromator,¹⁶ having a 600 grooves/mm concave holographic grating, blazed at 9000 Å of 2 Å resolution in the

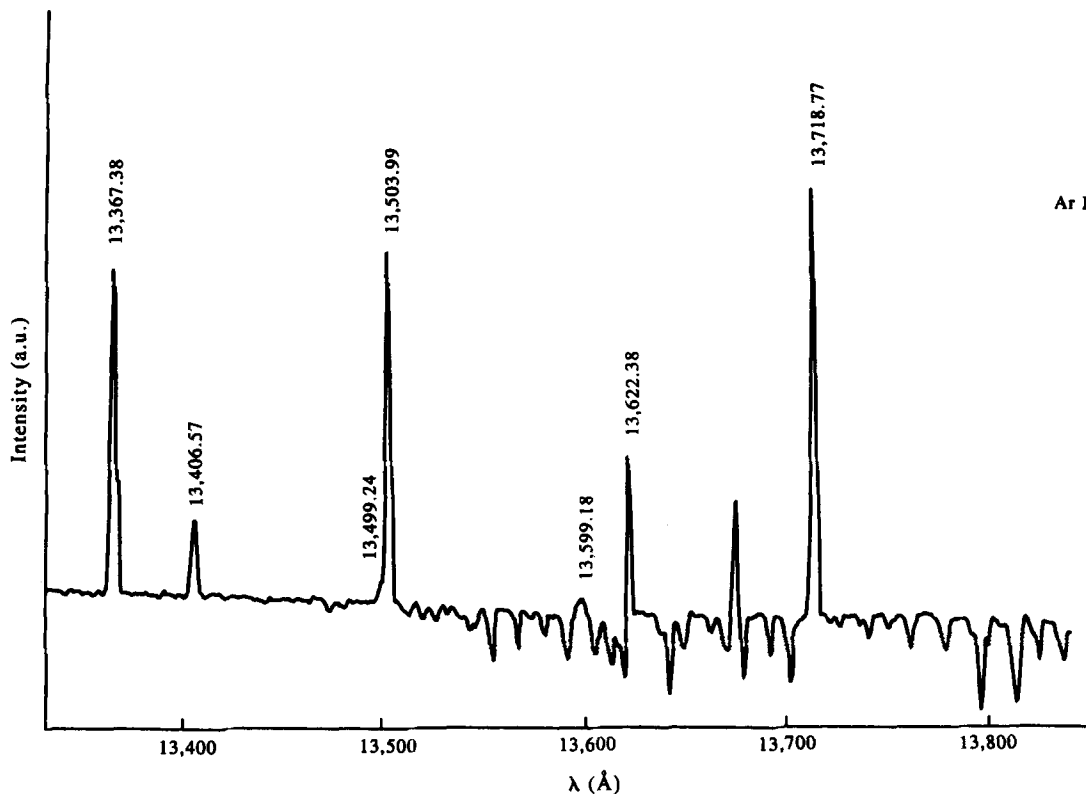


Fig. 1. Spectrum adjacent to the lines of Ar I, bands of water vapour which are in the collimator.

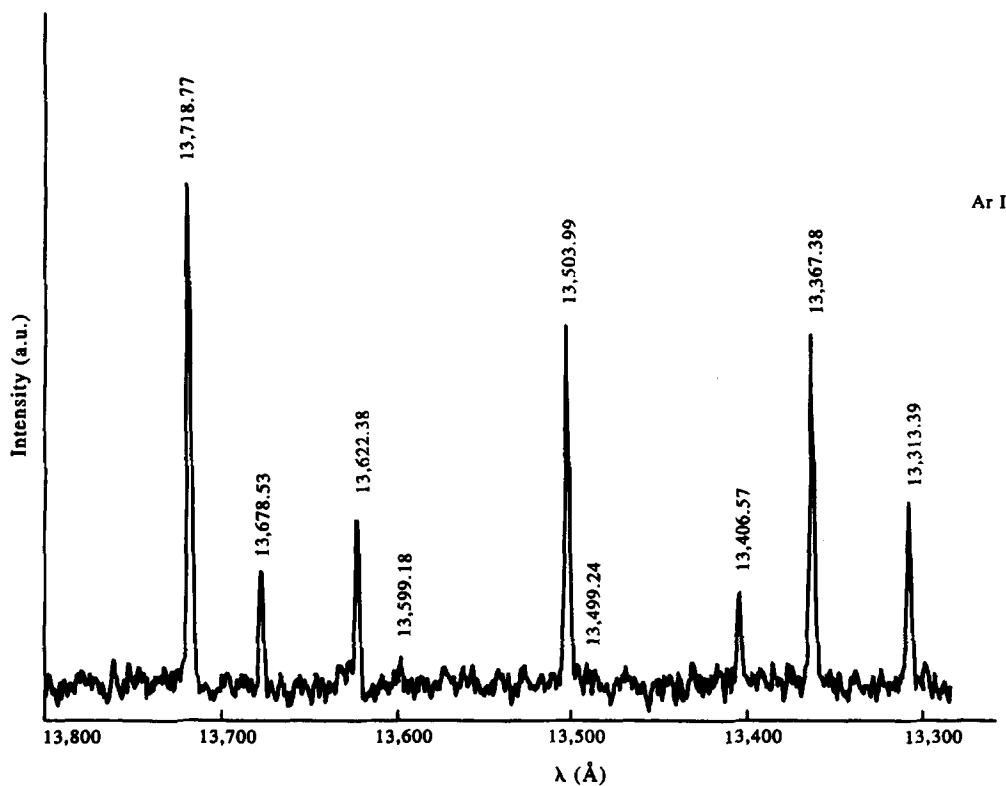


Fig. 2. Part of the spectrum of the Fig. 1, obtained with the Eagle monochromator and the InGaAs detector, in which the i.r. lines of Ar I are shown.

first order; appropriate cut-off optical filters were used to eliminate second-order radiation. Photons from 6000 to 11,000 Å were detected with an EMI 9898 B (S1 response) photomultiplier cooled with dry ice. Photons of the transition wavelength range, from 8000 to 15,000 Å, were detected with an InGaAs PIN photodiode (EPITAXX ETX 3000) operating in the photovoltaic mode; the photosensitive diameter was 3 mm.

To eliminate noise signals, a phase-sensitive detection technique^{5,17} was used; the i.r. light was chopped at a frequency of 450 Hz. The electronic system had consisted of a passband amplifier, an analog-digital converter and an analog phase-sensitive circuit which subtracts the half-periods of noise from the signal plus noise half-periods; the output of this circuit feeds a strip-chart recorder. The wavelength response of the spectrometric system was determined by using a calibrated tungsten-strip lamp; several emission spectra were recorded to obtain relative intensity with statistical uncertainties of 5%.

For the i.r. measurements, absorption bands due to water vapour in the ambient air between 13,400 and 14,700 Å, were avoided by inserting a drying compound into the monochromator (light path = 2 m); this situation can be appreciated in Figs. 1 and 2. The light path from the spectral source to the slit of the monochromator was only 5 cm; corrections due to this effect were negligible within the experimental error. The sensitivity of the detector system alloys measurements with optically-thin sources, avoiding systematic errors due to self-absorption; the Tl I and Ar I lines self-absorption tests were made by doubling the optical path by means of a mirror.

Absolute transition probabilities have also been obtained by combining our experimentally measured branching ratios with line-strength sum rules, viz.

$$\sum_j S_{jj'} = [(2J + 1)/(2I + 1)] \cdot I_{\max} \cdot |\int P_{nl}(r) \cdot r \cdot P'_{n'l'}(r) dr|^2$$

where $S_{jj'}$ is the line strength for $|nl, J\rangle \rightarrow |n'l', J'\rangle$ transitions and $\int P_{nl}(r) \cdot r \cdot P'_{n'l'}(r) dr$ is the single-electron radial integral.

Since Tl is a many-electron system having a relatively simple valence configuration ($6s^2 nl$), the radial wavefunctions $P_{nl}(r)$ were obtained by numerical integration of the radial Schrödinger equation including three terms in the Hamiltonian (Cowan⁹):

$$-\frac{\alpha^2}{2}(E - V)^2 - \frac{\alpha^2}{4}\left(\frac{dV}{dr}\right)r\frac{d}{dr}r^{-1} + \frac{\alpha^2}{2}\left(\frac{dV}{dr}\right)\frac{ls}{r},$$

Table 1. Transition probabilities for 7*p*-*ns*, 7*p*-*nd* and 6*d*-*np* lines of Tl I.

Transition levels		Absolute transition probabilities (10 ⁶ sec ⁻¹)				
		λ (Å)	Experimental	Theory		
Upper	Lower		This work	This work	Ref. 1	Ref. 4
9 <i>s</i> ² S _{1/2}	7 <i>p</i> ² P _{1/2} ^o	11,100.3	1.15 ± 0.11	1.08	1.18	1.26
	7 <i>p</i> ² P _{3/2} ^o	12,488.7	1.44 ± 0.14	1.49	1.40	1.46
10 <i>s</i> ² S _{1/2}	7 <i>p</i> ² P _{1/2} ^o	8976.7	0.38 ± 0.04	0.54	0.61	0.63
	7 <i>p</i> ² P _{3/2} ^o	9863.4	0.92 ± 0.09	0.80	0.74	0.72
11 <i>s</i> ² S _{1/2}	7 <i>p</i> ² P _{1/2} ^o	8129.9	0.34 ± 0.05	0.29	0.34	
	7 <i>p</i> ² P _{3/2} ^o	8850.5	0.42 ± 0.06	0.45	0.41	
7 <i>d</i> ² D _{3/2}	7 <i>p</i> ² P _{1/2} ^o	12,732.9	7.35 ± 0.62	8.19	5.30	5.10
	7 <i>p</i> ² P _{3/2} ^o	14,593.9	1.74 ± 0.15	1.14	1.31	1.30
8 <i>d</i> ² D _{3/2}	7 <i>p</i> ² P _{1/2} ^o	9509.4	3.25 ± 0.23	4.11	3.11	3.20
	7 <i>p</i> ² P _{3/2} ^o	10,510.7	1.19 ± 0.09	0.63	0.70	0.67
9 <i>d</i> ² D _{3/2}	7 <i>p</i> ² P _{1/2} ^o	8373.9	2.36 ± 0.16	2.36	1.90	
	7 <i>p</i> ² P _{3/2} ^o	9140.5	0.36 ± 0.02	0.37	0.40	
10 <i>d</i> ² D _{3/2}	7 <i>p</i> ² P _{1/2} ^o	7816.5	1.68 ± 0.18	1.47	1.21	
	7 <i>p</i> ² P _{3/2} ^o	8480.3	0.20 ± 0.01	0.23	0.25	
10 <i>p</i> ² P _{3/2} ^o	6 <i>d</i> ² D _{3/2}	10,072.1	0.059 ± 0.004	0.025	0.011	
	6 <i>d</i> ² D _{5/2}	10,156.0	0.17 ± 0.01	0.21	0.16	
11 <i>p</i> ² P _{3/2} ^o	6 <i>d</i> ² D _{3/2}	9257.4	0.019 ± 0.006	0.016	0.10	
	6 <i>d</i> ² D _{5/2}	9328.3	0.093 ± 0.014	0.11	0.095	

where α is the fine structure constant, E is the eigenvalue of the Schrödinger equation, l and s are orbital and spin angular-momentum operators and V is a semiempirical potential given for Green et al.,¹⁸ that includes core polarization effects,¹⁹ and incorporate the finite sites of nucleus.

The core polarization potential,

$$V_p(r) = -\frac{1}{2} \alpha_p \frac{r^2}{(r^2 + r_0^2)^3},$$

is included in the one-electron Hamiltonian of each valence electron. The static dipole polarizability, α_p , of Tl I is set to the value (39.33 a.u.) and r_0 is equated to the mean (2.38 a.u.) of the outermost (nlj) orbital of the unpolarized parent ion, calculated by Fraga et al.²⁰ The transition matrix element is corrected for core polarization by replacing the dipole moment operator of the valence electron by

$$D(r) = r[1 - \alpha_p(r^2 + r_0^2)^{-3/2}].$$

To incorporate the infinite site of the nucleus, the potential term is given for

$$V(r) = \frac{Z}{2R_0^3} r^2 - \frac{3}{2} \frac{Z}{R_0},$$

where R_0 is the radius of the nucleus.

Table 2. Transition probabilities for $3d \rightarrow 4p$ lines of Ar I.

Transition <i>jK</i> notation levels		Absolute transition probabilities (10 ⁶ sec ⁻¹)				
Upper	Lower	λ (Å)	Theory Ref. 10	Experiment		
				This work	Ref. 5	Ref. 11
$3d[3/2]_1$	$4p[1/2]_1$	9951.9		≤ 0.26	≤ 0.11	
	$4p[5/2]_2$	11,719.0	1.33	1.01 ± 0.08	0.8 ± 0.1	1.07
	$4p[3/2]_1$	12,402.8	9.26	10.70 ± 1.60	9.7 ± 0.8	11.50
	$4p[3/2]_2$	12,638.5	0.12	≤ 0.22	≤ 0.13	
	$4p[1/2]_0$	14,093.6	6.66	6.46 ± 1.00	5.9 ± 0.7	4.81
$3d[7/2]_3$	$4p[5/2]_3$	13,228.5	2.72	2.80 ± 0.42	2.5 ± 0.3	
	$4p[5/2]_2$	13,504.0	14.51	13.99 ± 1.10	14.9 ± 0.8	12.2
	$4p[3/2]_2$	14,739.1	0.17	0.20 ± 0.03	0.11 ± 0.20	0.099
$3d[5/2]_2$	$4p[1/2]_1$	10,722.2		≤ 0.13	0.14	
	$4p[5/2]_3$	12,544.4	0.35	0.21 ± 0.04	0.20 ± 0.07	0.14
	$4p[5/2]_2$	12,802.7	5.80	5.98 ± 0.59	6.3 ± 0.6	6.43
	$4p[3/2]_1$	13,622.4	11.33	10.41 ± 1.02	11.2 ± 0.8	8.19
	$4p[3/2]_2$	13,907.4	0.22	0.59 ± 0.09	0.34 ± 0.08	
$3d'[3/2]_2$	$4p[5/2]_3$	10,701.0	0.39	0.45 ± 0.07	0.40 ± 0.07	
	$4p[5/2]_2$	10,881.0	0.37	1.02 ± 0.15	0.9 ± 0.2	
	$4p[3/2]_1$	11,467.6	0.52	0.61 ± 0.06	0.58 ± 0.07	0.41
	$4p[3/2]_2$	11,668.7	4.43	6.30 ± 0.94	5.6 ± 0.8	4.23
	$4p'[3/2]_1$	13,023.3		0.30 ± 0.04	0.25 ± 0.07	
	$4p'[3/2]_2$	13,302.4		0.40 ± 0.04	0.30 ± 0.07	
	$4p'[1/2]_1$	13,678.5	12.36	14.29 ± 0.0	12.0 ± 0.7	6.96
$3d'[5/2]_2$	$4p'[3/2]_1$	13,313.4	15.39	15.53 ± 1.55	15.2 ± 0.8	14.6
	$4p'[3/2]_2$	13,599.2		2.55 ± 0.26	2.1 ± 0.2	2.54
	$4p'[1/2]_1$	13,992.6	0.02	≤ 0.2	≤ 0.05	
$3d'[3/2]_1$	$4p[1/2]_1$	8874.8		≤ 0.18	≤ 0.2	
	$4p[5/2]_3$	10,254.0	0.07	≤ 0.18	≤ 0.2	
	$4p[3/2]_1$	10,773.4	0.16	0.18 ± 0.02	0.22 ± 0.05	
	$4p[3/2]_2$	10,950.7	0.64	0.58 ± 0.06	0.57 ± 0.08	0.45
	$4p[1/2]_0$	12,026.6		0.56 ± 0.06	0.55 ± 0.08	0.47
	$4p'[3/2]_1$	12,139.8	3.34	6.51 ± 0.09	4.5 ± 0.5	5.14
	$4p'[3/2]_2$	12,377.2	0.34	0.43 ± 0.06	0.23 ± 0.05	
	$4p'[1/2]_1$	12,702.3	5.97	8.45 ± 1.00	7.2 ± 0.8	
	$4p'[1/2]_0$	15,046.5	6.25	6.41 ± 0.96	5.1 ± 0.6	5.81

Table 3. Transition probabilities for $5s \rightarrow 4p$ lines of Ar I.

Transition jK notation levels		Absolute transition probabilities (10^6 sec^{-1})				
Upper	Lower	λ (Å)	Theory Ref. 10	Experiment		
				This work	Ref. 6	Ref. 11
$5s[1/2]_0$	$4p[1/2]_1$	9291.6	2.82	4.0 ± 0.4	4.2 ± 0.6	3.66
	$4p[3/2]_1$	11,393.7	2.58	3.1 ± 0.3	3.5 ± 0.5	2.49
	$4p'[3/2]_1$	12,933.3	10.87	11.0 ± 1.0	11.9 ± 1.5	10.9
	$4p'[1/2]_1$	13,573.6	5.29	5.9 ± 0.9	5.4 ± 0.6	
$5s[3/2]_1$	$4p[1/2]_1$	10,478.1	1.9	2.7 ± 0.2	3.1 ± 0.5	1.9
	$4p[5/2]_2$	12,456.1	8.9	6.1 ± 0.6	10.4 ± 1.5	8.9
	$4p[3/2]_1$	13,230.9	4.6	2.9 ± 0.3		
	$4p[3/2]_2$	13,499.2	2.6	≤ 0.13	≤ 2.5	2.6
	$4p[1/2]_0$	15,172.3	1.3	1.0 ± 0.1	1.5 ± 0.3	
$5s[3/2]_2$	$4p[1/2]_1$	10,673.6	5.0	5.8 ± 0.9	5.8 ± 0.8	4.9
	$4p[5/2]_3$	12,487.6	10.3	13.5 ± 1.9	10.2 ± 1.5	10.3
	$4p[5/2]_2$	12,733.6	1.9	0.9 ± 0.1	1.4 ± 0.3	1.9
	$4p[3/2]_1$	13,543.8	0.5	0.5 ± 0.1	0.47 ± 0.01	0.48
	$4p[3/2]_2$	13,826.0	3.5	1.6 ± 0.2	1.4 ± 0.3	3.5

RESULTS AND DISCUSSION

The experimental transition probabilities of lines arising from the ($ns^2S_{1/2} \rightarrow 7p^2P_{1/2,3/2}$), ($nd^2D_{3/2} \rightarrow 7p^2P_{1/2,3/2}$) and ($np^2P_{3/2} \rightarrow 6d^2D_{3/2,5/2}$) transitions of Tl I are shown in Table 1; we include for comparison the theoretical values of Anderson et al¹ and Bardsley and Norcross,⁴ there is good agreement.

Transition probabilities obtained in the present work for lines arising from the Ar I $3d[3/2]_1$, $3d[7/2]_3$, $3d[5/2]_2$, $3d'[3/2]_2$, $3d'[5/2]_2$, $3d'[3/2]_1$ levels, in jK notation, are given in Table 2; we include for comparison the experimental values of Tanarro⁵ and Wiese.¹¹ Table 3 shows the experimental transition probabilities of lines arising from the Ar I $5s'[1/2]_0$, $5s[3/2]_1$, $5s[3/2]_2$ levels; we include for comparison the experimental values of Tanarro⁶ and Wiese.¹¹ Table 4 shows the values of the transition probabilities of lines arising from the Ar I $4p[1/2]_1$, $4p[5/2]_2$, $4p[3/2]_1$, $4p[3/2]_2$, $4p'[3/2]_1$,

Table 4. Transition probabilities for $4p \rightarrow 7s$ lines of Ar I.

Transition jK notation levels		Absolute transition probabilities (10^6 sec^{-1})				
Upper	Lower	λ (Å)	Theory Ref. 10	Experiment		
				This work	Ref. 13	Ref. 12
$4p[1/2]_1$	$4s[3/2]_2$	9122.9	17.42	16.01 ± 2.40		18.9 ± 0.7
	$4s[3/2]_1$	9657.8	4.65	6.07 ± 0.91		5.43 ± 0.43
	$4s'[1/2]_0$	10,470.0	0.86	1.06 ± 0.1		0.98 ± 0.15
	$4s'[1/2]_1$	11,488.1	0.17	0.21 ± 0.04		0.19 ± 0.06
$4p[5/2]_2$	$4s[3/2]_2$	8014.8	9.80	10.47 ± 1.57	10.6 ± 1.3	9.28 ± 0.24
	$4s[3/2]_1$	8424.6	20.80	21.44 ± 3.22	22.3 ± 2.7	21.5 ± 1.07
$4p[3/2]_1$	$4s[3/2]_2$	7723.8	5.65	5.20 ± 0.78	4.9 ± 0.8	5.18 ± 0.26
	$4s[3/2]_1$	8103.7	25.70	25.7 ± 3.8	24.3 ± 2.9	25.00 ± 1.25
	$4s'[1/2]_0$	8667.9	2.60	3.00 ± 0.45	2.9 ± 0.3	2.43 ± 0.19
	$4s'[1/2]_1$	9354.2	0.90	1.22 ± 0.18	1.3 ± 0.2	1.06 ± 0.08
$4p[3/2]_2$	$4s[3/2]_2$	7635.1	27.00	27.99 ± 4.20	23.8 ± 2.8	24.5 ± 1.96
	$4s[3/2]_1$	8006.2	4.90	8.34 ± 1.40	7.1 ± 0.8	4.9 ± 0.7
$4p'[3/2]_1$	$4s[3/2]_2$	7147.0	1.00	0.91 ± 0.13	0.7 ± 0.1	0.62 ± 0.05
	$4s[3/2]_1$	7471.2	0.10	≤ 0.1	0.03 ± 0.01	0.02 ± 0.002
	$4s'[1/2]_0$	7948.2	20.40	18.88 ± 2.83	18.7 ± 2.1	18.6 ± 1.4
	$4s'[1/2]_1$	8521.4	13.40	14.63 ± 2.19	15.7 ± 1.7	13.9 ± 1.1
$4p'[3/2]_2$	$4s[3/2]_2$	7067.2	4.50	4.53 ± 0.62	4.2 ± 0.5	3.8 ± 0.3
	$4s[3/2]_1$	7383.9	9.20	10.52 ± 1.57	9.5 ± 1.0	8.47 ± 0.68
$4p'[1/2]_1$	$4s[3/2]_2$	6965.4	7.40	7.00 ± 1.05	6.3 ± 0.7	6.39 ± 0.32
	$4s[3/2]_1$	7727.9	1.90	2.10 ± 0.31	1.8 ± 0.2	1.83 ± 0.09
	$4s'[1/2]_0$	7724.2	12.50	12.10 ± 1.81	11.7 ± 1.9	11.70 ± 0.58
	$4s'[1/2]_1$	8264.5	17.20	15.80 ± 1.37	16.5 ± 1.8	15.30 ± 0.76

$4p'[3/2]_2$ and $4p'[1/2]_1$ levels; we include the experimental values of Wiese¹² and Borge¹³ for comparison. The experimental errors of relative transition probabilities given in Tables 1–4 are the result of statistical uncertainties ($\sim 5\%$) and uncertainties in the spectral response determination ($\sim 5\%$).

The present results are also compared in Tables 2, 3 and 4 with the theoretical values of Lilly,¹⁰ which were obtained by using the same Coulomb approximation and intermediate-coupling scheme. In general, there is agreement with previously published experimental values and good agreement with the calculations of Lilly.

In summary, in the present measurements, results have been obtained for Ar I that differ by $\sim 10\%$ from the mean experimental values and for Ti I, the results differ by 10–15% from the mean theoretical values; for these infrared lines there are no published experimental studies.

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REFERENCES

1. E. M. Anderson, E. K. Anderson, and V. F. Trusov, *Opt. Spectrosc. (URSS)* **22**, 471 (1967).
2. J. Migdalek, *Can. J. Phys.* **54**, 118 (1976).
3. D. V. Neuffer and E. D. Commins, *Phys. Rev.* **A16**, 844 (1977).
4. J. N. Bardsley and D. W. Norcross, *JQSRT* **23**, 575 (1980).
5. I. Tanarro and J. Campos, *JQSRT* **36**, 345 (1986).
6. I. Tanarro and J. Campos, *Can. J. Phys.* **63**, 1389 (1985).
7. C. Peraza, P. Martín, and J. Campos, *JQSRT* **45**, 63 (1991).
8. J. M. Bridges and W. L. Wiese, *Phys. Rev.* **A2**, 285 (1970).
9. R. D. Cowan, *The Theory of Atomic Structure and Spectra*, p. 422, Univ. of California Press, Los Angeles, CA (1981).
10. R. A. Lilly, *JOSA* **66**, 245 (1976).
11. W. L. Wiese, J. M. Bridges, R. N. Kornblith, and D. E. Kelleher, *JOSA* **59**, 1206 (1969).
12. W. L. Wiese, J. W. Brault, K. Danzmann, V. Helbig, and M. Kock, *Phys. Rev.* **A39**, 2461 (1989).
13. M. J. G. Borge and J. Campos, *Physica* **119C**, 359 (1983).
14. C. E. Moore, *Atomic Energy Levels, NMS 467*, Vol. 11c, U.S.GPO, Washington, DC (1958).
15. C. Peraza, P. Martín, and J. Campos, *JQSRT* **46**, 455 (1991).
16. P. Martín, M. Ortiz, and J. Campos, *An. Fis.* **B85**, 70 (1989).
17. M. L. Meade, *J. Phys. E: Sci. Instrum.* **15**, 395 (1982).
18. A. E. S. Green, D. L. Sellin, and A. S. Zachor, *Phys. Rev.* **184**, 1 (1969).
19. J. Migdalek and W. E. Baylis, *J. Phys. B: Atom. Molec. Phys.* **12**, 2595 (1979).
20. S. Fraga, J. Karwowski, and K. M. S. Saxena, *Handbook of Atomic Data*, pp. 323, 469, Elsevier, New York, NY (1976).